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Group velocity interpretation of the stability theory of Gustafsson, Kreiss, and Sundström

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Abstract. The existing stability theory for finite difference models of hyperbolic initial boundary value problems, due to Gustafsson, Kreiss, and Sundström, is difficult to understand in its original algebraic formulation. Here we show that the GKS stability criterion has a physical interpretation in terms of group velocity: if the finite difference model together with its boundary conditions can support a set of waves at the boundary with group velocities pointing into the field, then it is unstable. A simple argument explains why such a set of waves is unstable, and yields a new theorem on what kind of unstable growth to expect. We give examples in one and two space dimensions.

Key words and phrases: finite difference method, partial differential equation, initial boundary value problem, stability, group velocity

AMS(MOS) subject classifications: 65M10, 73D99

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0. INTRODUCTION

When time-dependent partial differential equations are solved numerically by finite difference methods, more boundary conditions are usually required than the physics of the problem provides. This necessitates a selection of additional numerical boundary conditions, and in this choice an overriding consideration is numerical stability. For the case of hyperbolic equations, the stability question is solved in principle by the theory of Gustafsson, Kreiss, and Sundström [9]—henceforth "GKS". However, application of this theory has been hindered by its complexity and abstractness. The purpose of this paper is to point out that the main result of the GKS theory has a simple physical interpretation in terms of group velocity. This interpretation does not provide an alternative to the algebraic stability test of the GKS theory, which may in practice be difficult to carry out, but it makes the meaning of the algebra clear. It also leads to a proof that except for certain borderline cases, GKS-unstable models are unstable not only in the complicated norm of [9], but in the ℓ_2 norm also.

Group velocity is a concept associated with energy propagation under dispersive equations, not hyperbolic ones. Its significance to numerical stability results from the fact that finite difference models, even of nondispersive equations, are necessarily dispersive. A general discussion of group velocity effects in finite difference models may be found in [13]. For this one should also see the work of R. Vichnevetsky, including [15] and the papers referenced there. The particular topic of the present paper is treated in much greater detail in the author's PhD dissertation, [14].

In the first section here, we look at a simple example to illustrate the group velocity idea. Section 2 extends this to the general setting of GKS. Section 3 applies these results to define certain general classes of unstable difference models, in several space dimensions as well as one, which generalize examples that have appeared in the literature.

1. AN EXAMPLE

Consider the model problem

$$u_t = u_x \tag{1.1}$$

for $x \in (-\infty, \infty)$, $t \in [0, \infty)$, with initial conditions

$$u(x, 0) = f(x). \tag{1.2}$$

Such an initial-value problem on a domain without boundary is called a *Cauchy problem*. The exact solution is $u(x,t) = f(x+t)$, a leftward translation at speed 1.

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In a Fourier or normal mode analysis of (1.1), one looks for wave solutions

$$u(x,t) = e^{i(\omega t - \xi x)}, \tag{1.3}$$

where ω is the (temporal) ***frequency*** and ξ is the ***wave number***. Eq. (1.1) implies that ω and ξ are related by

$$\omega = -\xi, \tag{1.4}$$

which is called the ***dispersion relation*** of (1.1).

Let us set up a uniform grid with space step h and time step k, and approximate $u(x,t)$ by a grid function v_j^n:

$$v_j^n \approx u(jh, nk), \qquad (-\infty < j < \infty, \quad n \geq 0).$$

One of the simplest difference models for (1.1) is the ***leap frog (LF)*** formula

$$v_j^{n+1} = v_j^{n-1} + \lambda(v_{j+1}^n - v_{j-1}^n), \tag{1.5}$$

where λ is the ***mesh ratio*** or ***Courant number*** k/h. For $\lambda < 1$ this scheme is stable; we say that LF is ***Cauchy stable.*** By plugging (1.3) into (1.5), one obtains the dispersion relation for LF,

$$e^{i\omega k} = e^{-i\omega k} + \lambda\left[e^{-i\xi h} - e^{i\xi h}\right],$$

that is,

$$\sin \omega k = -\lambda \sin \xi h. \tag{1.6}$$

This relation approximates (1.4) only for small ωk and ξh—that is, only for waves that are well resolved on the grid.

Since ω is no longer a linear function of ξ, the LF model is said to be ***dispersive.*** According to a theory going back to Lord Rayleigh [3,4,11,16], energy associated with wave number ξ will propagate at a ***group velocity**** given by

$$C = \frac{d\omega}{d\xi}. \tag{1.7}$$

For LF one obtains, by differentiating (1.6) implicitly,

$$C = -\frac{\cos \xi h}{\cos \omega k}. \tag{1.8}$$

It is apparent that energy associated with different wave numbers or frequencies will travel at different group velocities, so that an initial signal that is not monochromatic will change form as it propagates. For a well resolved wave one has $\xi h \approx 0$ and

*The group velocity is not the same as the phase velocity, $c = \omega/\xi$. Readers unfamiliar with this distinction are encouraged to read the discussions in [4], [11], or [16].

$\omega k \approx 0$, hence $\omega k \approx -\lambda \xi h$ by (1.6), and (1.8) becomes

$$C = -1 + \frac{1-\lambda^2}{2}(\xi h)^2 + O((\xi h)^4). \tag{1.9}$$

Thus typical signals travel leftward at a speed less than the ideal speed 1, with higher wave numbers lagging more than lower ones. This dispersion of wave numbers gives rise to the spurious oscillations near discontinuities that are familiar in finite difference computations. Alternately, if one sets up a wave packet consisting of energy at essentially constant ω and ξ, the packet will be seen to move leftward without changing at the velocity (1.8)≈(1.9). For illustrations see [13,15].

The key to our analysis is that (1.8) is valid not only for well resolved waves, but for all waves supportable on the grid, which means a range of $(-\pi, \pi]$ in both ξh and ωk. In fact for many waves, C has the wrong sign, so that energy travels *in the wrong direction*. In particuar, (1.8) gives the following group velocities for four extreme situations—the constant function and three *parasitic waves* that are sawtoothed in x and/or t:

	$(\xi h, \omega k)$	C
(a)	$(0,0)$	-1
(b)	$(\pi,0)$	1
(c)	$(0,\pi)$	1
(d)	$(-\pi,\pi)$	-1

Line (b) implies, for example, that if initial data are supplied to LF of the form

$$v_j^0 = v_j^1 = \begin{cases} (-1)^j & (jh \le \epsilon) \\ 0 & (jh > \epsilon) \end{cases} \tag{1.10}$$

for some $\epsilon \gg h > 0$, then the result as t increases will be a steady rightward motion of the wave front from $x = \epsilon$ at speed 1. See Fig. 6 of [13].

Now let us turn to an initial boundary value problem. Let (1.1) and (1.2) be given on the quarter-plane $x, t \ge 0$; no boundary data at $x = 0$ are needed to make this problem well posed. To obtain an approximate solution on the grid $j, n \ge 0$, we can specify initial values v_j^0 and v_j^1 for $j \ge 0$, and apply LF for $n \ge 2$ at points $j \ge 1$. An additional boundary formula is then needed for u_0^n, $n \ge 2$.

Suppose we (foolishly) pick the boundary formula

$$v_0^{n+1} = \frac{1}{2}(v_0^n + v_2^n) \qquad (n \ge 1) \tag{1.11}$$

and proceed to step forward in time. Now imagine that at some time step a perturbation (e.g. rounding error) happens to be introduced that has the form (1.10). It is easy to see that such a wave satisfies (1.11), and therefore this mode will behave just as if the domain were still $(-\infty, \infty)$: the wave front will begin to propagate rightwards

n = 1

t = .0125

n = 4

t = .05

n = 40

t = .5

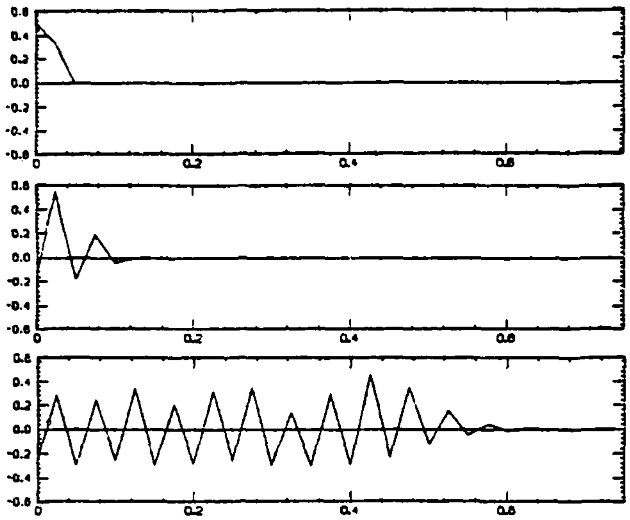

FIG 1. Appearance of an unstable rightgoing parasitic wave in the Leap Frog model (1.5), (1.11) with initial conditions (1.12).

into $x \geq 0$ at speed 1. The initial perturbation, with sum-of-squares energy on the order of ϵ, will give rise to a growing solution with energy on the order of $\epsilon + t$. Since ϵ might be arbitrarily small, this amounts to an amplification of the initial perturbation by an unbounded factor. *The difference scheme is unstable, because there exists a rightgoing wave that satisifies both the interior formula (1.5) and the boundary condition (1.11).*

One can verify experimentally that the scheme (1.5), (1.11) is susceptible to an unstable rightgoing mode of type (b). Fig. 1 shows a computation on a grid with $h = 1/40$, $\lambda = 1/2$. For initial data we took $v_j^0 = v_j^1 = 0$ for all j except for the "random" nonzero initial values

$$v_1^0 = 1, \qquad v_0^1 = \frac{1}{2}, \qquad v_1^1 = \frac{1}{3}. \tag{1.12}$$

Figs. 1a–c show the resulting solution at steps $n = 1, 4, 40$, i.e. $t = .0125, .05, .5$. Obviously the expected mode has been excited, and apparently no others. In a realistic computation, rounding errors would cause a similar radiation of energy in this mode from the boundary. From (1.8) one can see that there are many other rightgoing modes for LF—in fact, any wave with $\xi h < \pi/2$ and $\omega k > \pi/2$ or $\xi h > \pi/2$ and $\omega k < \pi/2$. Mode (c) is the simplest example. None of these lead to instabilities, however, because none of them satisfy (1.11).

The main GKS theorem asserts, roughly, that an initial boundary value problem model is stable if and only if

(i) the interior difference formula is Cauchy stable;

(ii) the model (including boundary conditions) admits no eigensolutions that grow

from each time step to the next by a constant factor z with $|z| > 1$;

(iii) the model (including boundary conditions) admits no wavelike solutions with group velocity $C \geq 0$.

In practice, (i) is easy to verify, and there are rarely any growing modes of type (ii). The critical condition is therefore (iii). We will state the GKS theory more precisely in the next section.

To obtain stability in the present example, we might replace (1.11) by the condition

$$v_0^{n+1} = \frac{1}{2}(v_0^n + v_1^n). \tag{1.13}$$

Then it is not hard to verify that (ii) is satisfied, and the only wavelike mode admitted by the difference model is $(\xi h, \omega k) = (0, 0)$, which has $C = -1 < 0$, hence cannot cause radiation from the boundary. Thus (iii) is satisfied and the model is stable.

It may seem that the kind of energy growth in Fig. 1 is too weak to be dangerous, and should not be considered unstable. Though this may be true for the present model problem, it is usually not true in realistic computations, for various reasons. One is that when a rightgoing signal of constant amplitude can occur, then sometimes similar signals with amplitudes growing linearly with n or faster are also possible. Such noise might soon become significant even though it began at the level of rounding error. Second, if the semiinfinite region $x \geq 0$ is replaced by a bounded strip such as $[0, 1]$, then a wavelike instability of type (iii) may be converted by repeated reflections back and forth to an exponential growth of type (ii), which is unambiguously unstable. Third, the rate of growth may also be increased if variable coefficients or lower order (undifferentiated) terms are present. The GKS theory shows that by ruling out the relatively weak instability of Fig. 1, one can be certain that these more serious effects are also excluded.

In summary, GKS instability amounts to the spontaneous radiation of energy from the boundary into the interior. In a realistic physical application, this is likely to cause trouble.

2. GENERAL STATEMENT OF THE GKS THEORY

Consider now a first-order hyperbolic system

$$\frac{\partial}{\partial t}u(x,t) = A\frac{\partial}{\partial x}u(x,t), \tag{2.1}$$

where u is an N-vector and A is a constant nonsingular Hermitian matrix of dimension $N \times N$. (All of what follows extends to equations that include a zeroth-order term $Bu(x,t)$ and a forcing function $F(x,t)$.) Let (2.1) be modeled in $x \geq 0$ by a fixed $s+2$-level Cauchy stable difference formula, explicit or implicit, whose stencil extends ℓ points to the left and r points to the right of center. For example, LF has $s = 1$ and $\ell = r = 1$. We can write the difference model formally as

$$Q_{-1}v^{n+1} = \sum_{\sigma=0}^{s} Q_\sigma v^{n-\sigma}, \tag{2.2}$$

where $v_j^n \approx u(jh, nk)$ is an N-vector for each j and n, and each Q_σ is a difference operator with matrix coefficients of size $N \times N$. For simplicity we will assume that each Q_σ is constant, independent of h. If (2.2) is applied for $j \geq \ell$, then boundary formulas are required to determine values v_j^n for $j = 0, \ldots, \ell - 1$:

$$v_j^{n+1} = S_j(\{v_i^{n-s}\}_{0\leq i\leq q}, \ldots, \{v_i^n\}_{0\leq i\leq q}, \{v_i^{n+1}\}_{\ell\leq i\leq q}) \qquad 0 \leq j \leq \ell - 1. \tag{2.3}$$

These formulas comprise both physical boundary conditions, such as couplings between outflowing and inflowing components of v, and additional purely numerical boundary conditions. Unfortunately, it would take many pages to state precisely the form of the difference model and the assumptions it must satisfy, so for details the reader is referred to §1 and §5 of [9] and to §4 of [6], where the presentation is clearer.

The GKS idea is to perform a *normal mode analysis* of what solutions the model (2.2), (2.3) can support. To find the normal modes, let us begin by ignoring the boundary conditions (2.3). In the last section, we looked for wavelike solutions (1.3) with frequency ω and wave number ξ. Let us now write

$$z = e^{i\omega k}, \qquad \kappa = e^{-i\xi h}. \tag{2.4}$$

The vector analog of (1.3) then takes the form

$$v_j^n = z^n \kappa^j \psi, \tag{2.5}$$

where ψ is a constant nonzero N-vector. Now suppose that instead of taking $|z| = 1$, we let z be any complex number with $|z| > 1$. Then there are still modes of the form (2.5), but now κ will become complex also, with $|\kappa| \neq 1$. (The circumstance $|z| > 1$, $|\kappa| = 1$ would violate the von Neumann condition, and we have assumed that (2.2)

FIG 2. Sketch of signals $v_j^n = \kappa^j z^n$ with $|z| > 1$.
(a) Rightgoing, $|\kappa| < 1$. (b) Leftgoing, $|\kappa| > 1$.

is Cauchy stable.) Figure 2 suggests the two possibilities $|\kappa| < 1$ and $|\kappa| > 1$. From one time step to the next, each mode in Figure 2 increases in amplitude by a ratio $|z|$. It is obvious, however, that we may view this equivalently as a lateral motion, rightward in case (a) and leftward in case (b), combined with a change of phase. We will call these *rightgoing* and *leftgoing* modes, respectively.

Modes of the form (2.5) do not always span the set of solutions with time dependence z^n. If $p > 1$ κ's coalesce for some z, then a defective situation results in which a p-parameter collection of modes are possible,

$$v_j^n = z^n \kappa^j j^d \psi \qquad (0 \le d \le p-1). \tag{2.6}$$

(The defective situation $p > 1$ rarely occurs in practice.) A fundamental lemma of [9] now states

Proposition *([9], Lemma 5.2). For any z with $|z| > 1$, (2.2) admits a total of exactly $N\ell$ linearly independent solutions of type (2.6) with $|\kappa| < 1$, and exactly Nr such solutions with $|\kappa| > 1$.* ∎

This result is proved by reducing the difference model to a recurrence relation in j. From it we get the general solution to (2.2) that varies with z^n:

Proposition. *For any z with $|z| > 1$, the general solution to (2.2) of the form $v_j^n = z^n \phi_j$ may be written*

$$z^n \phi_j = z^n \sum_{|\kappa(z)|<1} \sum_{d=0}^{p_\kappa - 1} \alpha_{\kappa,d} \kappa^j j^d \psi_\kappa + \sum_{|\kappa(z)|>1} \sum_{d=0}^{p_\kappa - 1} \alpha_{\kappa,d} \kappa^j j^d \psi_\kappa \tag{2.7}$$

for arbitrary constants $\alpha_{\kappa,d}$. ∎

We may think of (2.7) as describing a linear combination of $N\ell$ rightgoing and Nr leftgoing modes.

Now let us reintroduce the boundary conditions. The full model can support only any solutions (2.7) that satisfy (2.3) as well as (2.2). There are $N\ell$ boundary formulas, and (2.7) depends on $N(\ell + r)$ free parameters, so one may expect that there will normally be an Nr-dimensional space of solutions that the model supports. In such a solution, a combination of leftgoing waves hits the boundary and reflects as a combination of rightgoing waves. This kind of configuration is in general not unstable, even though the reflected energy may be larger than the incident energy. But occasionally it may happen that some collection of rightgoing signals satisfies (2.2) and (2.3) by itself, i.e. without any stimulation by leftgoing signals. In this case the left/right reflection coëfficient has become infinite. Then the model has an instability of the *Godunov-Ryabenkii (G-R)* type [12]:

Godunov-Ryabenkii theorem. *Suppose that for some z with $|z| > 1$, the model (2.2), (2.3) admits a solution of the form*

$$z^n \phi_j = z^n \sum_{|\kappa|<1} \sum_{d=0}^{p_\kappa - 1} \alpha_{\kappa,d} \kappa^j j^d \psi_\kappa. \tag{2.8}$$

Then it is unstable.

Proof. If $v_j^\sigma = z^\sigma \phi_j$ is taken as initial data for $0 \le \sigma \le s$, the solution as n increases will be $v_j^n = z^n \phi_j$ for all n. Since $t = nk$, this means that v will grow like $|z|^{t/k}$. With $|z| > 1$ this growth is unbounded for any t as $k \to 0$. ∎

A similar solution made up of leftgoing waves would of course also grow unboundedly in amplitude, but this would amount to propagation of energy leftward from infinity rather than generation of energy at the boundary. The initial wave would not have finite size in ℓ_2 or any other reasonable norm, and could not be excited by rounding errors or other perturbations. The wave ϕ in (2.8), on the other hand, does belong to ℓ_2, and is called an ***eigensolution*** of the difference model.

The set of potential eigensolutions ϕ, since they are made up of rightgoing signals only, is spanned by $N\ell$ free parameters, which exactly matches the number of boundary conditions (2.3). Therefore the G-R condition has this algebraic form: does there exist, for any $|z| > 1$, a nontrivial solution of a system of $N\ell$ linear homogeneous equations in $N\ell$ unknowns that depends on z? Hence the problem can be cast as a *determinant condition* involving an $N\ell \times N\ell$ matrix $M(z)$. (For examples see [5,6,9].)

Godunov-Ryabenkii theorem (determinant condition). *A necessary condition for stability of the model (2.2), (2.3) is*

$$\det M(z) \neq 0 \tag{2.9}$$

for all z with $|z| > 1$. ∎

A virtue of normal mode analysis is that in principle, the determinant condition can be verified mechanically, although in practice this may be very difficult [6]. In contrast, stability proofs by the energy method [10,12] require a measure of intuition and luck.

The limitation of the G-R condition is that it is a necessary condition for stability, but far from sufficient. To obtain a condition that is sufficient or nearly so, one must investigate the borderline case $|z| = 1$. This is the main achievement of the GKS theory. From the GKS point of view, this investigation is a matter of showing algebraically that certain resolvent estimates obtained for $|z| > 1$ extend continuously to $|z| = 1$. From our point of view, it is a matter of observing that the ideas of "leftgoing" and "rightgoing" still make sense as $|z| \to 1$, because in the limit $|z| = 1$ the lateral motion in Figure 2 becomes a group velocity.

First, the GKS approach. For $|z| = 1$, what unstable solutions along the lines of (2.7), but also including components with $|\kappa| = 1$, can (2.2), (2.3) support? The GKS theory gives the following answer based on a ***perturbation test.*** First, one can rule out components with $|\kappa| > 1$, as before. One then investigates: are there any solutions to (2.2) and (2.3) of the form (cf. (2.8))

$$z^n \phi_j = z^n \sum_{|\kappa| \le 1} \sum_{d=0}^{p_\kappa - 1} \alpha_{\kappa,d} \kappa^j j^d \psi_\kappa \tag{2.10}$$

for some z with $|z| \ge 1$? If not, the model is stable. If so, a further test is required. Given a solution (2.10), let z be perturbed slightly to a new value $\tilde{z}$ with $|\tilde{z}| > 1$. Each κ with $|\kappa| = 1$ will then move to a nearby value $\tilde{\kappa}$ with $|\tilde{\kappa}| \ne 1$. If every κ for which $\alpha_{\kappa,d} \ne 0$ in (2.10) moves to $|\tilde{\kappa}| < 1$, then (2.10) is an unstable mode and the model is unstable. A solution ϕ of this sort with $|z| = 1$ and $|\kappa| = 1$ for at least one κ is called a ***generalized eigensolution*** of the difference model. The qualification "generalized" has been introduced because such a solution no longer belongs to ℓ_2.

The GKS stability theorem can now be stated:

GKS stability theorem. *The model (2.2), (2.3) is stable if and only if (2.2) and (2.3) admit no eigensolutions or generalized eigensolutions with $|z| \ge 1$.* ∎

A simpler but less constructive way to express the same theorem is by means of the determinant condition. The $N\ell \times N\ell$ matrix $M(z)$, which for $|z| > 1$ embodies the condition that there be an eigensolution of G-R type, has a continuous extension to $|z| = 1$. Let $M(z)$ for $|z| \ge 1$ denote this extension. Then one has:

GKS stability theorem (determinant condition.) *A necessary and sufficient condition for stability of the model (2.2), (2.3) is*

$$\det M(z) \ne 0$$

for all z with $|z| \ge 1$.

Proof. This result is stated as Lemma 10.3 and the sentence following in [9]. ∎

Now for the group velocity interpretation. Assume, as is usually the case, that $\tilde{\kappa}$ depends analytically on $\tilde{z}$ in a neighborhood of a point z where $|\kappa(z)| = |z| = 1$. By (2.4), we have then

$$d\tilde{z} = ikz\, d\omega, \qquad d\tilde{\kappa} = -ih\kappa\, d\xi$$

and therefore

$$C = \frac{d\omega}{d\xi} = -\frac{d\tilde{z}/ikz}{d\tilde{\kappa}/ih\kappa} = -\frac{1}{\lambda}\frac{d\tilde{z}/z}{d\tilde{\kappa}/\kappa}. \tag{2.11}$$

If $C > 0$, (2.11) implies that $d\tilde{z}/z$ and $d\tilde{\kappa}/\kappa$ will have equal and opposite signs. In other words, κ moves inside the unit circle when z moves outside. Conversely, if $C < 0$, κ moves outside the circle when z does, and the solution (2.10) does not represent a generalized eigensolution. Thus *the GKS perturbation test for generalized eigensolutions corresponds to a test for positive group velocities.*

The argument of the example in Section 1 explains why a solution made of waves with positive group velocities should be unstable. The same idea leads naturally to the following necessary condition for stability in the general case:

Theorem 1. *Suppose that the model (2.2), (2.3) admits a solution of the form (2.10) with $|z| = 1$, where for each κ with $|\kappa| = 1$, the group speed defined by (2.11) exists and satisfies $C_\kappa \geq 0$. Suppose that for at least one such κ, say κ_0, $C_{\kappa_0} > 0$. Then the model is unstable.* ∎

In fact, we can be more precise:

Theorem 2. *Suppose that the model (2.2), (2.3) admits an unstable generalized eigensolution as described in Thm. 1. Then there exists a constant $\rho > 0$ such that if $\epsilon > 0$ and $t \geq 0$ are arbitrary, then for all sufficiently small h, k, there exists a set of intitial data $\{v^\sigma\}$, $0 \leq \sigma \leq s$, such that*

$$|v_j^\sigma| \leq 1 \qquad \text{for } j \geq 0, \quad 0 \leq \sigma \leq s,$$

$$v_j^\sigma = 0 \qquad \text{for } jh > \epsilon, \quad 0 \leq \sigma \leq s,$$

and

$$\|v^{t/k}\|_2^2 \geq \rho t, \tag{2.12}$$

where $\|\ \|_2$ denotes the norm defined by

$$\|v\|_2^2 = h\sum_{j=0}^{\infty} |v_j|^2.$$

Proof. Assume $d = 0$ for all waves in (2.10). Let initial data be chosen equal to $1/\alpha_{\max}$ times (2.10) near $x = 0$, but cutting off smoothly to 0 for $jh > \epsilon$. As time elapses, each smooth wave front will propagate rightwards at its group speed

C_κ. This will cause growth at least as fast as (2.12) if ρ is taken as $C_{\kappa_0}|\alpha_{\kappa_0}|/|\alpha_{\max}|$. For a more rigorous proof, including the case $d > 0$, see [14]. ∎

Theorems 1 and 2 are not quite the same as the GKS stability theorem. The latter asserts that even if every wave in (2.10) has $C = 0$, the model is still unstable. From the group velocity point of view, it is not clear why this should be so, for if a cut off wave is set up as in the proof of Thm. 2, but with $C = 0$ for each component, then as t increases the wave front will approximately remain stationary. The explanation is that the GKS theorem does not define stability in terms of a simple ℓ_2 norm, but in a more complicated fashion under which a wave that remains stationary at the boundary turns out to be *unstable* (Defn. 3.3 of [9]). The GKS definition has other peculiarities too, the most troublesome of which is that it defines stability not in terms of a norm at a fixed time t, but in terms of an integral of the solution over all $t > 0$. We will not go into the details.

The situation here is something like that discussed at the end of Section 1: by choosing a conservative definition of stability, one can obtain a theory that is robust with respect to variable coefficients, undifferentiated terms, and so on. In fact, the striking difference between the GKS theorem and our Thm. 1 (coupled with the G-R condition) is that the former gives a necessary *and sufficient* condition for stability, made possible by the use of the complicated norm. The difference between this situation and that of Section 1 is that in this case it is not as clear that in realistic computations, the conservative choice is generally necessary. We are now dealing with a borderline subcase ($C = 0$) of a borderline case (wavelike eigensolutions). There do not appear to be any published examples of instabilities of the $C = 0$ type in which numerical trouble actually becomes evident.

In practice, stability for a particular problem will be determined by a host of interacting phenomena that depend on whether and how smoothly the coefficients vary, whether an undifferentiated term is present, whether homogeneous or inhomogeneous boundary data are supplied, whether there is more than one boundary, and whether the boundaries are characteristic. Probably no simple theory can encompass all permutations of such effects without some artificiality. For a further discussion of these matters, see [14].

3. APPLICATIONS

We will now give five examples of unstable boundary conditions, or their equivalents. In each case the unstable mode consists of nothing more than a combination of constant and sawtoothed signals, and this is typical for instabilities encountered in practice. In the course of the examples we will extend the theory to problems with interfaces and to multidimensional problems, where a vector group velocity becomes needed.

Because of the repeated occurence of sawtoothed waves, it is convenient to devise a name for schemes under which they propagate in the wrong direction:

Defn. Let Q be a scalar difference formula. Suppose that whenever Q admits a solution $v_j^n = z^n$ with $|z| = 1$ and group speed $C \in \mathbb{R}$, then it also admits the solution $v_j^n = (-1)^j z^n$, and this wave has group speed $C' \in \mathbb{R}$ satisfying $CC' \leq 0$. Then Q is ***x*-reversing.** Likewise if the existence of a solution $v_j^n = \kappa^j$ with $|\kappa| = 1$ and group speed C implies the existence of a solution $v_j^n = (-1)^n \kappa^j$ with $CC' \leq 0$, then Q is ***t*-reversing.**

Any scheme based on the standard second-order centered difference in x or t is reversing for that variable, with $CC' = -1$. Thus LF, CN (Crank-Nicolson), and BE (Backwards Euler) are x-reversing, and LF and LF4 (fourth-order leap frog) are t-reversing, as is any modification of LF with (spatial) dissipation added. More generally, the general $(2\ell+1)$-point difference approximation to $\partial/\partial x$ or $\partial/\partial t$ of order 2ℓ is also reversing [14], with $CC' < -1$ for $\ell \geq 2$. A dissipative scheme cannot be x-reversing, and a scheme that dissipates oscillations in t (for which there is no name) cannot be t-reversing [14].

Application 1: space extrapolation with *t*-reversing formulas

Let (1.1) be modeled by a difference formula Q for $j \geq \ell$ coupled with *q_jth-order space extrapolation* boundary conditions

$$S: \qquad [(E-1)^{q_j} v^{n+1}]_j = 0 \qquad (0 \leq j \leq \ell - 1)$$

for the boundary points, where E is the shift operator defined by $[Ev]_j = v_{j+1}$ and $q_j \geq 1$ for each j. The result appears in [9], and in various other papers, that S is unstable if $\ell = 1$ and the interior scheme is LF. Here is a generalization:

Theorem 3. *Any consistent t-reversing difference formula Q for (1.1), such as LF or LF4 with or without dissipation, is unstable in combination with the boundary condition S.*

Proof. The sawtoothed wave $v_j^n = (-1)^n$ satisfies S for any set $\{q_j\}$, and if Q is t-reversing, it also satisfies Q and has $C > 0$, since by consistency $v_j^n \equiv 1$ must satisfy Q with $C = -1 < 0$. By Thm. 1, the model is therefore unstable. ∎

The instability with S of an LF scheme with spatial dissipation added is pointed out by Goldberg and Tadmor in [8].

Application 2: "one-sided leap frog" with t-reversing formulas

Similarly, it has been noted in various papers that if (1.1) is modeled by LF for $j \geq 1$ with the boundary condition

$$v_0^{n+1} = v_0^{n-1} + 2\lambda(v_1^n - v_0^n),$$

then the result is GKS-unstable. As a generalization, consider any set of boundary conditions

$$v_j^{n+1} = v_j^{n-1} + 2kD_jv_j^n \qquad 0 \leq j \leq \ell - 1, \tag{3.1}$$

where each D_j is a one-sided spatial difference operator involving at most j points to the left of center, consistent with $\partial/\partial x$. We obtain just as above

Theorem 4. *Any consistent t-reversing difference formula Q for (1.1) is unstable in combination with the boundary condition (3.1).* ▮

Application 3: sign-changing coefficients; nonlinear instability

Consider the problem

$$u_t = \begin{cases} a_-u_x & (x < 0) \\ a_+u_x & (x > 0), \end{cases} \tag{3.2}$$

where a_- and a_+ are constants. To model this by finite differences, we might set up a grid $((j + \frac{1}{2})h, nk)$ for $-\infty < j < \infty$, $n \geq 0$. Suppose we apply consistent difference formulas Q_- and Q_+ for $x \leq -h/2$ and $x \geq h/2$, respectively, taking no special measures to improve accuracy at the interface. The stability question for such an interface is essentially the same as for an initial boundary value problem, and the GKS theory has been applied to such problems by Kreiss, Ciment, Oliger, and others [5]. Formally, a scalar model including an interface can be "folded" into an initial boundary-value problem for a system of two variables, and then the GKS theory is directly applicable. What is really going on in such a process is a search for eigensolutions or generalized eigensolutions consisting of waves that are *outgoing* from the point of view of the interface. That is, *a difference model involving a scheme- or mesh-change interface is GKS-stable if and only if there is no eigensolution of the kind suggested in Fig. 3:*

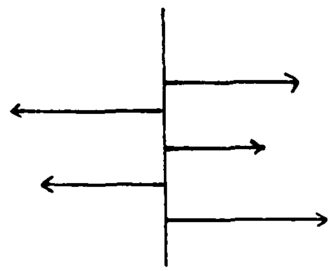

FIG 3. In a problem containing an interface, a solution consisting of a set of outgoing waves on each side will be unstable.

If $\operatorname{sgn} a_- = \operatorname{sgn} a_+$, then most models for (3.2) are stable, but stability vanishes if $\operatorname{sgn} a_- \neq \operatorname{sgn} a_+$:

Theorem 5. *Let (3.2) be modeled by consistent formulas Q_- and Q_+ as indicated above. If $a_- > 0 > a_+$, the model is unstable. If $a_- < 0 < a_+$ and Q_- and Q_+ are both x-reversing or both t-reversing, the model is also unstable.*

Proof. In the first case, the constant function $v_j^n \equiv 1$ is an outgoing wave that satisfies all the difference formulas, so the model is unstable by Thm. 1. In the second case, the same goes for a space or time sawtooth $(-1)^j$ or $(-1)^n$. ∎

This elementary example is related to certain known examples of ***nonlinear instability***. If the Burgers equation

$$u_t = uu_x$$

is modeled by the LF scheme

$$v_j^{n+1} - v_j^{n-1} = \lambda v_j^n (v_{j+1}^n - v_{j-1}^n),$$

then exponentially growing instabilities arise that are characterized by oscillations of the form [7,10]

$$v_j^n \approx 0, \quad v_{j+1}^n < 0, \quad v_{j+2}^n > 0, \quad v_{j+3}^n \approx 0.$$

Though it is easy to enough to examine this problem directly, it also has a rough interpretation along GKS lines. LF is an x-reversing formula, and the instability observed looks approximately like the outgoing sawtooth of Thm. 5 from the point of view of the sign-change interface at $x_{j+3/2}$. The linear growth of this outgoing wave would be converted into exponential by reflection at points x_j and x_{j+3} even if the coefficients v_j did not change from one time step to the next; the fact that they do makes the growth even more rapid.

Application 4: mesh refinement

In problems where the solution is smoother in some regions than in others, it may be useful to combine grids of various sizes [5]. Where two such grids meet, some kind of interface condition will be required. Here is a mesh refinement scheme for which the stability result takes a particularly interesting form (Joseph Oliger, private communication). Suppose that for $x \geq 0$, the grid $x_j = hj$ $(j \geq 0)$ is set up, while for $x \leq 0$, this is coarsened by an integral factor of $m \geq 2$, so that the grid is $x_j = mhj$ for $j \leq 0$. If (1.1) is modeled by LF for $j \leq -1$ and $j \geq 1$, a formula is still needed to determine v_0^n. The obvious choice is to apply the coarse grid LF formula at $j = 0$, which is possible because the value required at $x = mh$ is available from the fine grid:

$$v_0^{n+1} = v_0^{n-1} + m\lambda(v_m^n - v_{-1}^n). \tag{3.3}$$

Now suppose a wave is considered of the form

$$v_j^n = \begin{cases} (-1)^j & (j \geq 0), \\ 1 & (j \leq 0). \end{cases} \tag{3.4}$$

On $x \leq 0$, this wave is constant and has $C = -1$. On $x \geq 0$, it is sawtoothed and has $C > 0$ since LF is x-reversing. Thus (3.4) is outgoing on both sides of the interface. Moreover *if m is even,* it obviously satisfies (3.3), so we have instability.

This conclusion can be generalized as follows:

Theorem 6. *Let (1.1) be modeled by a consistent x-reversing 3-point formula on $x_j = jh$ for $j \geq 1$ coupled with any consistent formula on $x_j = jmh$ for $j \leq 0$, with right-hand values for the latter near the interface taken where needed from points imh with $i \geq 1$. Then if m is even, the model is unstable.* ∎

For LF or CN the sawtooth (3.4) turns out to be the only instability that arises, so this kind of mesh refinement is stable if m is odd.

Application 5: two-dimensional problems

Abarbanel and Gottlieb [1] and Abarbanel and Murman [2] have studied the stability of various difference schemes for the following problem in two space dimensions:

$$u_t = u_x + u_y \qquad x, t \geq 0, \quad y \in (-\infty, \infty). \tag{3.5}$$

The solutions to this equation consist of functions

$$u(x, y, t) = u(x + t, y + t, 0).$$

That is, information propagates with a vector velocity $(-1, -1)$. Since the flow is outward across the boundary $x = 0$, no boundary conditions should be given there.

For a multidimensional problem like this, ξ becomes a wave number vector $\boldsymbol{\xi}$, and the group speed (1.7) generalizes to a vector ***group velocity*** given by

$$\boldsymbol{C} = \nabla_{\boldsymbol{\xi}}\omega, \tag{3.6}$$

where $\nabla_{\boldsymbol{\xi}}$ denotes the gradient with respect to $\boldsymbol{\xi}$. As in the one-dimensional case, difference schemes not only lead to incorrect group speeds, but may cause propagation in the wrong direction—which means at any angle in the (x, y) plane whatsoever. See [13] for a discussion with examples. In two dimensions, Thm. 1 becomes: *if a difference model of (3.5) admits a solution consisting of waves with group velocity $\boldsymbol{C}$ pointing into $x \geq 0$ (i.e. with $C_x \geq 0$), it is unstable.* If one such wave has $C_x > 0$, then unbounded growth in ℓ_2 will take place, as in Thm. 2.

For example, suppose (3.5) is modeled by the leap frog formula

$$v_{ij}^{n+1} - v_{ij}^{n-1} = \lambda(v_{i+1,j}^{n} - v_{i-1,j}^{n}) + \lambda(v_{i,j+1}^{n} - v_{i,j-1}^{n}). \tag{3.7}$$

The dispersion relation for this scheme is

$$\sin\omega k = -\lambda\sin\xi h - \lambda\sin\eta h,$$

where $\boldsymbol{\xi} = (\xi, \eta)$, and from (3.6) there follow the group velocity components

$$C_x = -\frac{\cos\xi h}{\cos\omega k}, \qquad C_y = -\frac{\cos\eta h}{\cos\omega k}.$$

As usual, these reduce to the ideal value $\boldsymbol{C} = (-1, -1)$ for ξh, $\omega k \approx 0$. If we look at parasites, on the other hand, we see that a sawtooth form in x or y negates C_x or C_y, respectively, and a sawtooth in t negates both. One has

	$\xi h, \eta h, \omega k$	$\boldsymbol{C}$
(a)	$(0,0,0)$, (π,π,π)	$(-1,-1)$
(b)	$(\pi,0,0)$, $(0,\pi,\pi)$	$(+1,-1)$
(c)	$(0,\pi,0)$, $(\pi,0,\pi)$	$(-1,+1)$
(d)	$(\pi,\pi,0)$, $(0,0,\pi)$	$(+1,+1)$

Thus parasites can travel in any of the directions at 45° to the grid. If any parasite of form (b) or (d) is permitted by the boundary conditions, the difference model is unstable.

Abarbanel et al. consider various boundary formulas. Four of these are ***space extrapolation*** and ***skewed space extrapolation***,

S: $\qquad (E_x - 1)^q v_0^{n+1} = 0,$

SS: $\qquad (E_x E_y - 1)^q v_0^{n+1} = 0,$

and ***space/time extrapolation*** and ***skewed space/time extrapolation***,

ST: $\qquad (E_x E_t^{-1} - 1)^q v_0^{n+1} = 0,$

SST: $\quad (E_x E_y E_t^{-1} - 1)^q v_0^{n+1} = 0.$

Here E_x, E_y, and E_t denote the shift operators in x, y, and t. By counting sign changes, one can see which boundary formulas permit which sawtooths. One finds

	stable sawtooths	*unstable sawtooths*
S	$(0,0,0),(0,\pi,0)$	$(0,0,\pi),(0,\pi,\pi)$
SS	$(0,0,0),(\pi,\pi,\pi)$	$(0,0,\pi),(\pi,\pi,0)$
ST	$(0,0,0),(0,\pi,0),(\pi,0,\pi),(\pi,\pi,\pi)$	
SST	$(0,0,0),(\pi,0,\pi)$	$(0,\pi,\pi),(\pi,\pi,0)$

Thus *S, SS, and SST are all unstable with LF.* It turns out that ST, which we see has no sawtooth instabilities, is indeed stable.

Other difference formulas typically permit fewer sawtooths, hence are stable with more boundary conditions. Let us generalize to d space dimensions. If κ and j are d-vectors, κ^j will denote $\kappa_1^{j_1}\cdots\kappa_d^{j_d}$.

Defn. Let Q be a scalar difference formula in d space dimensions. Suppose that whenever Q admits a solution $v_j^n = \kappa^j z^n$ with $|z| = |\kappa_i| = 1$ for each i, $\kappa_I = 1$ for some I, and group velocity $C \in R^d$, then it also admits the solution $v_j^n = (-1)^I \kappa^j z^n$, and this wave has group velocity $C' \in R^d$ satisfying $C'_i = C_i$ for $i \neq I$ and $C_I C'_I \leq 0$. Then Q is **x_I-reversing.** Suppose that whenever Q admits a solution $v_j^n = \kappa^j$ with $|\kappa_i| = 1$ for all i and group velocity $C \in R^d$, then it also admits the solution $v_j^n = \kappa^j(-1)^n$, with group velocity $C' \in R^d$ satisfying $C_i C'_i \leq 0$ for $1 \leq i \leq d$. Then Q is **t-reversing.**

Now let Q be a difference model of

$$u_t = \sum_{j=1}^{d} u_{x_j}$$

on $t, x_1 \geq 0$, $x_j \in (-\infty, \infty)$ for $2 \leq j \leq d$, and let the boundary conditions S, SS, ST, SST be extended in the obvious way. By the same arguments as above we obtain the following theorem:

Theorem 7. *The following assertions hold in the stated direction only; their converses are not in general valid.*

(i) The model S,Q is unstable if Q is t-reversing.

(ii) The model SS,Q is unstable if Q is t-reversing or if Q is x_1-reversing and also x_j-reversing for at least one $j \geq 2$.

(iii) The model SST,Q is unstable if Q is x_1-reversing and/or t-reversing, and also x_j-reversing for at least one $j \geq 2$. ∎

Among the formulas Q considered by Abarbanel et al. are multidimensional versions of LF, CN, BE, and MC (MacCormack's scheme). One sees readily that LF is t-

reversing and x_j-reversing for each j, CN and BE are x_j-reversing for each j but not t-reversing, and MC is not reversing in any variable. It turns out that all combinations of these schemes with S, SS, ST, or SST that are not ruled unstable by Thm. 7 are in fact stable.

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